Effects of Crystal Twinning on the Solution of the Macromolecular Structure Using MAD

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The crystal structure of gpD, the capsid-stabilizing protein of bacteriophage λ, was solved by multiwavelength anomalous diffraction (MAD) for a selenomethionine (SeMet) derivative of the protein at 1.8 Å resolution, using crystals in space group $P2_1$. Subsequent analysis showed that the crystals of both the original protein and the SeMet derivative were pseudo-merohedrally twinned with a twinning fraction ~0.36, due to the near-identity of the *a* and *c* axes. Although examples of twinned crystals solved by Molecular Replacement are known, no twinned structures have been solved by MAD technique. We have analyzed the crystal structure solution, discussed the utility of twinned crystals for solving the structure using MAD and of different phasing strategies, and compared the results obtained with several software packages using the original and de-twinned data.